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Experimental and Numerical Investigation of the Role of Initial Condition of the Dynamics of Rayleigh-Taylor Mixing

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Masters Thesis Proposal

Experimental and Numerical Investigation of the Role of Initial Conditions on the Dynamics of Rayleigh-Taylor Mixing

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Abstract

Experiments and direct numerical simulations have been performed to examine the effects of initial conditions on the dynamics of a Rayleigh-Taylor mixing layer. Experiments were performed on a water channel facility to quantify the interfacial and velocity perturbations initially present at the two-fluid interface in a small Atwood number mixing layer. The measurements have been parameterized for implementation in numerical simulations of the experiment, and two- and three-dimensional direct numerical simulations (DNS) of the experiment have been performed. It is shown that simulations implemented with initial velocity perturbations are required to match experimentally-measured statistics. Data acquired from both the experiment and numerical simulations are used to elucidate the role of initial conditions on the evolution of integral-scale, turbulence, and mixing statistics. Early-time turbulence and mixing statistics will be shown to be strongly dependent upon the early-time transition of the initial perturbation from a weakly- to a strongly-nonlinear flow.

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1. Introduction

An experimental and numerical investigation examining the role of initial conditions on buoyancy-driven turbulence will be conducted. In this study, buoyancy-driven turbulence is generated by the Rayleigh-Taylor instability, which occurs in an unstable stratification of a heavy fluid with density ρ_1 above a lighter fluid with density ρ_2, in a gravitational field g (Rayleigh 1884; Taylor 1950). The Rayleigh-Taylor instability occurs when the density and pressure gradients are oriented such that $\nabla\rho \cdot \nabla p < 0$ (Chandrasekhar 1961). As the instability develops and nonlinear processes begin to dominate, a turbulent mixing layer develops between the two fluids.

Rayleigh-Taylor flows represent one of the few canonical fluid flows that encapsulate the laminar, transition and turbulent regimes. The development of a complete understanding of Rayleigh-Taylor instability-generated turbulence is important because of the broad impact such flows have in nature and in technological applications. In astrophysical flows, it is hypothesized that the limiting factor in the creation of heavy elements in collapsing stars is the growth of the mixing layer formed by the adverse stratification of densities in the stars gravitational field (Smarr et al. 1981). Many deep-sea ocean currents and atmospheric flows contain Rayleigh-Taylor generated mixing and turbulence. Also, the growth of a Rayleigh-Taylor driven mixing layer has been shown to be the limiting factor in the effective yield of inertially-confined fusion target capsules (Lindl 1998).

Modeling such complicated flows, which contain an ever-expanding range of timescales and length-scales, represents a grand challenge for the turbulence community. Validation of more predictive turbulent transport models of anisotropic, inhomogeneous, variable-density turbulence and mixing require a priori knowledge of correlations, such as $\overline{u_i u_j}$, $\overline{\rho u_j}$ and $\overline{u_i u_j u_k}$, in order to validate models for unclosed terms. Currently, there are no models describing the effects of initial conditions on the development of the growth of a turbulent Rayleigh-Taylor driven mixing layer. Even less is known about the effects of the initial conditions of a flow on the fluctuating turbulent quantities and molecular mixing within the mixing layer.

2. Objectives

The principal objectives of this research are:

- Experimentally measure the initial density and velocity perturbations at the two-fluid interface of a Rayleigh-Taylor mixing layer, including the first measurements of spanwise perturbations;
- Parameterize the measured initial density and velocity conditions so that they may be implemented in numerical simulations of the experiment;
- Perform two- and three-dimensional direct numerical simulations (DNS) of the experiment using high-accuracy numerical schemes so that all viscous and mass diffusion scales are resolved;
- Examine turbulence and mixing statistics from both numerical and experimental results to elucidate the role of initial conditions in the early-time transition of the mixing layer.

This work is motivated by the desire to validate and to further develop turbulent transport and mixing models of variable-density, buoyancy-driven flows. Validation of such models requires knowledge of the internal structure of fluctuating quantities within the mixing layer and how the initial conditions affect their temporal evolution. The development of transport models for such complicated flows is required to avoid the computational expense of DNS for the higher Reynolds numbers flows of interest.

The experimental portion of this work will be completed using an existing water channel facility at Texas A&M University. Details of the experimental configuration and diagnostics will be given in a later section. The numerical portion of this investigation will use a high-accuracy spectral/compact difference code developed at the Lawrence Livermore National Laboratory to simulate the experiment. Details of the numerical scheme and implementation of the initial conditions will also be presented in a later section.

3. Background

In the presence of small perturbations at the two-fluid interface in a Rayleigh-Taylor unstable flow, each mode grows exponentially according to linear theory (Chandrasekhar 1961). Each mode continues to grow independently until nonlinear dynamics begin to dominate the formation of the mixing layer. Modes begin to interact nonlinearly, such that smaller modes merge to create larger buoyant structures. Secondary Kelvin-Helmholtz instabilities grow as localized areas of high shear develop between rising bubbles and falling spikes. As the mixing layer becomes turbulent and grows in spatial extent, it has been shown using dimensional analysis that (under appropriate conditions) the only relevant length-scale is gt^2, such that the width of the mixing layer is modeled as $h = \alpha A g t^2$ in a self-similar regime, where $A \equiv (\rho_1 - \rho_2)/(\rho_1 + \rho_2)$ is the Atwood number and α is dimensionless (Anuchina et al. 1978; Youngs 1984). Buoyancy-driven turbulence provides an efficient mixing mechanism for miscible fluids.

In the interest of determining which factors influence the growth and internal structure of a Rayleigh-Taylor mixing layer, there exist numerous experiments and even more numerical simulations on the subject. Within the experimental community, a common issue is the lack of control over the initial seeding of the perturbations and the inability to fully quantify the initial conditions in all directions. Similarly, numerical simulations are either initialized with ad hoc initial perturbations or utilize some form of partially-measured (typically one-dimensional) initial conditions. An overview of the major contributions to the field will be presented here.

3.1. Related Experiments

The first single-mode Rayleigh-Taylor instability experiments were performed by Taylor (1950) using a vertical tube containing fluids having different densities. Emmons et al. (1960) accelerated a tank on rails to generate an unstable interface between methanol and air. Read (1984) performed the first significant measurements of the growth of a mixing layer seeded with a multi-mode perturbation using a drop tank accelerated downward by rocket motors. This experiment allowed for high accelerations and a large range of Atwood numbers, but allowed for no measurement of the initial conditions or internal structure of the mixing layer. In a similar experiment, Dimonte & Schneider (1996) used the linear electric motor (LEM) facility at the Lawrence Livermore National Laboratory to accelerate a drop tank, producing an unstable interface between fluids. While more experimental control and diagnostics were available for the LEM experiments, only a qualitative description and estimate of the initial perturbations was possible.

Other experiments include the overturning of a tank containing two fluids of different densities (Andrews 1986; Andrews & Spalding 1990). Linden et al. (1994) and Dalziel et al. (1999) produced an unstable interface by withdrawing a plate from a tank that contained a heavier fluid above a lighter fluid. Both experimental techniques allowed for some quantification of the initial conditions. Dalziel et al. used a particle tracking method to measure the velocity perturbation introduced by the withdrawal of the splitter plate. Numerical simulations performed by Dalziel et al. will be reviewed in the following section.

Ramaprabhu & Andrews (2004a) used the same water channel configuration proposed for the current experiments to measure both large-integral-scale and small-scale statistics. Due to the extended data collection times, statistical convergence of velocity and density spectra, double and triple correlations were capable of being measured. Of particular interest is the ability to measure the initial density and velocity fluctuations at the two-fluid interface. The numerical simulations that implement the measured initial conditions will be reviewed in the following section.

3.2. Related Simulations

Youngs (1984) performed monotone-integrated large eddy simulations (MILES) (Boris et al. 1992; Pope 2000) of two-dimensional, incompressible, miscible Rayleigh-Taylor instability-generated turbulence using an Eulerian hydrodynamics code. Youngs' early simulations were aimed at determining the growth of single- and multi-mode perturbations: he showed that simulations implemented with only high-wavenumber velocity perturbations did not grow as fast in the later stages of development as similarly initialized simulations that included a low-wavenumber interfacial perturbation. Youngs (1991) performed three-dimensional (128^3 grid points) simulations with isotropic, multi-mode interfacial perturbations. Youngs continued the theme of examining the late-time growth rate of the mixing layer with respect to the determination of an asymptotic value of α in the equation for the self-similar growth of a mixing layer. Youngs also addressed the issue of the structure and evolution of internal fluctuating quantities, in particular density fluctuations and molecular mixing. Youngs (1994) presented similar findings with higher resolution ($160^2 \times 270$).

Using the same numerical method as Youngs (1991; 1994), Dalziel et al. performed three-dimensional simulations ($160 \times 80 \times 200$) of the plate-withdrawal experiment described previously. Dalziel et al. also showed that an irrotational (potential flow) model of the initial velocity perturbations generated better agreement between experiments and simulations than the use of interfacial perturbations alone. However, several factors prevented direct comparison between experiment and simulation. The experiments were performed with $A = 2.0 \times 10^{-3}$, while the simulations implemented $A = 9.1 \times 10^{-2}$, for numerical stability reasons. Also, the numerical simulations utilized a Schmidt number, $Sc \equiv D/\nu \sim 1$, while the experiments had $Sc \sim 1000$. Finally, the three-dimensional numerical simulations did not include any measured perturbations in the spanwise direction. With this method of initialization it is not clear to what degree the initial seeding in the second homogeneous direction affects the early-time structure and transition of the mixing layer.

Cook & Dimotakis (2001) performed $256^2 \times 1024$ DNS of Rayleigh-Taylor mixing with A = 0.5 and Sc = 1 to examine how initial conditions affect the asymptotic growth of the mixing layer and the evolution of the degree of molecular mixing within the layer. All initial conditions implemented assumed isotropic interfacial perturbations within an annulus of wavenumbers, assuming a Gaussian distribution about a particular mode number of interest. Cook & Zhou (2002) increased the resolution of the DNS to $512^2 \times 2040$ to examine the transfer of energy between scales of motion (Cabot et al. 2004). Under the assumption that the memory of the initial conditions can be neglected in the late-time growth regime, Cook et al. (2004) used a very high-resolution large-eddy simulation (1152^3) to further investigate the asymptotic growth of a mixing layer and the late-time mixing transition (Dimotakis 2000).

Dimonte et al. (2004) also studied how the initial conditions affect the asymptotic growth rate of a Rayleigh-Taylor mixing layer. Dimonte et al. performed a simulation study employing a variety of numerical schemes using spatial resolutions of $128^2 \times 256$ and $256^2 \times 512$. The initial isotropic interfacial perturbations were initialized with an approximately uniform distribution of energy in either modes 16-32 or 32-64 so that all of the simulations would evolve in the limit of strong mode-coupling. Dimonte et al. demonstrate a lower-bound value of $\alpha \approx 0.03$ when mode-coupling is the only mechanism for the development of larger scales.

Ramaprabhu & Andrews (2004b) used measured density and velocity fluctuations to perform numerical simulations of the water channel experiment (Ramaprabhu & Andrews 2004a). Ramaprabhu and Andrews (2004b) used an Eulerian MILES code (Andrews 1984; Dimonte 2004) to investigate how well numerical simulations initialized with density and velocity perturbations agree with experimentally-measured mixing layer growth rates and fluctuating quantities. Instead of implementing the one-dimensional measurement in one direction within the simulation and assuming a perturbation in the other direction, they assumed isotropic initial perturbations in all homogeneous directions. The three-dimensionality of the flow was seeded by rotating the one-dimensional density or velocity spectrum in wavenumber space to create a two-dimensional perturbation. It was found that simulations with velocity perturbations matched closer with experimental measurements of growth rates and fluctuating quantities than simulations using interfacial perturbations alone.

4. Description of Experiments

The experimental objectives of this research will be accomplished using an existing water channel facility at Texas A&M University (Snider & Andrews 1994; Wilson & Andrews 2002; Ramaprabhu & Andrews 2004a). The water channel is an open-loop device in which cold and warm water ($\Delta T \approx 5°$ C) enter the channel initially separated by a thin Plexiglas splitter plate. The density difference between the two streams is induced by the thermal expansion of the warmer fluid. Upon entering the mixing section of the channel, an adverse density stratification occurs and mixing ensues. The water channel is supplied by two 500-gallon water tanks and has a running time on the order of ten minutes. Previous researchers have shown the water channel measurements to be statistically-stationary for higher-order moments of velocity fluctuations and density fluctuations. Figure 1 shows a schematic of the water channel and its diagnostic capabilities.

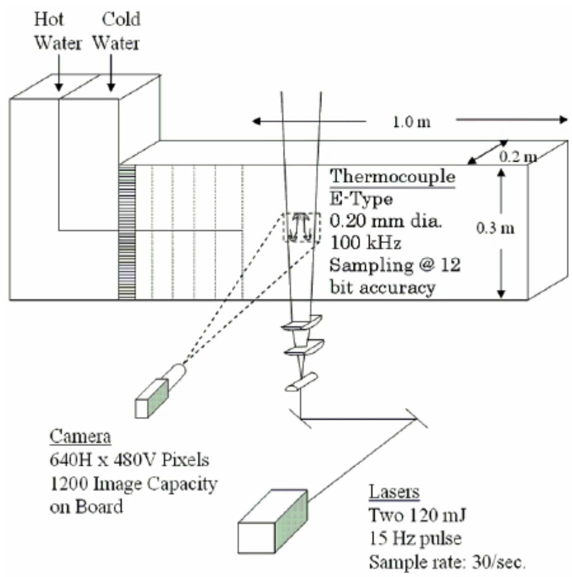

Figure 1. Schematic of the experimental setup. For reference, the x-axis is in the direction of the mean channel flow, the y-axis is in the spanwise direction, and the z-axis is in the direction of gravity.

Three separate, independent measurements will be made to quantify the initial conditions of the flow. First, the fluctuating density field off the trailing-edge of the splitter plate will be measured using high-resolution thermocouples. Velocity perturbations in the streamwise direction will be measured using particle image velocimetry (PIV). Finally, the interfacial perturbation in the spanwise direction will be measured using planar laser-induced fluorescence (PLIF). Further details of each experimental method are given below.

Density perturbations will be measured streamwise (x-direction) using new high-resolution E-type thermocouples positioned at $x = 0.1$ and $x = 1.0$ cm downstream from the splitter plate. The new thermocouples have a smaller weld bead diameter, resulting in a much less intrusive diagnostic and improving spatial resolution. The spatial resolution enhancements are desirable so that the uncertainty on mixing statistics and scalar fluctuations spectra are reduced. Temperature measurements will be converted to density values using an equation of state for water (Kukulka 1981). Given a value of the diffusion layer thickness between the two fluids, it will be shown that the density perturbation may be transformed into an interfacial perturbation. Initial mixing statistics and the structure of the interfacial perturbation spectrum will be analyzed.

Velocity perturbations in the streamwise direction will be measured using particle image velocimetry (PIV) (Adrian 1991). A series of conical lenses will create a sheet of laser light in the xz-plane of the water channel. The laser sheet will be positioned so that u and w velocity measurements may be made at a point just off the splitter plate. The vertical fluctuating velocity w' will be used to reconstruct the momentum perturbation at the two-fluid interface. The small, but finite, velocity deficit located immediately after the trailing-edge of the splitter plate will also be included as measured by the u velocity profile in the vertical direction. All measurements of the initial velocity perturbations will be conducted with both fluid streams at the same temperature to remove buoyancy-generated effects from the wake dynamics.

Cross-stream measurements will be made by arranging a sheet of laser light normal to the mean flow direction. Rhodamine 6G dye will be introduced so that the top (cold) stream fluoresces in the presence of laser light. Images of the fluorescing dye will allow the two-fluid interface in the cross-stream direction to be reconstructed and parameterized. For these experiments, the optical axis of the camera will not coincide with the direction normal to the laser sheet, thus introducing perspective errors into the recorded image; special consideration will be given to the process of dewarping the images (Pratt 1991; van Oord 1997). These spanwise measurements are novel in the following way. These are the first experiments to employ off-axis imaging on the water channel, and these are the first measurements of the initial seeding in the spanwise direction of a Rayleigh-Taylor flow.

5. Description of Direct Numerical Simulations

The numerical objectives of this research will be completed using a spectral/compact finite-difference code developed at Lawrence Livermore National Laboratory primarily for direct and large-eddy simulation of Rayleigh-Taylor generated turbulence (Cook & Dimotakis 2001; Cook et al. 2004). The code solves the mass, momentum and species diffusion equations on a Cartesian grid. For the present investigation, the code will be used to perform DNS, in which the entire range of scales is resolved within a turbulent flow. Spatial derivatives are computed by spectral methods in the homogeneous x- and y-directions and 10^{th}-order compact finite-differencing in the inhomogeneous z-direction. Time is advanced using a 3^{rd}-order Adams-Bashforth-Moulton scheme for all timesteps with the exception of the first, which employs a forward Euler scheme. To avoid complicated inflow and outflow boundary conditions, the numerical simulations will have no mean flow component. Boundary conditions in the homogeneous directions will be periodic and no-slip/no-penetration in the vertical direction. The code is parallelized with MPI and is tuned for use on large-scale computing facilities across many processors.

DNS will be performed to determine the optimum method of parameterization of the measured initial conditions. Simulation parameters will be chosen such that they match the experimental values of density, viscosity, mass (thermal) diffusivity, and physical domain size. A summary of the simulations to be performed and their respective initial conditions is given in Table 1.

Initial Conditions	x-direction perturbation	y-direction perturbation
2D Density	Thermocouple (density)	
3D Density	Thermocouple (density)	PLIF (density)
2D Velocity	PIV (velocity)	
3D Velocity	PIV (velocity)	PLIF (density)

Table 1. Summary of DNS.

For the implementation of the initial conditions in each simulation, each perturbation will be taken from the power spectra of the respective experimental measurement. The interfacial perturbation in the x-direction will be obtained from the thermocouple measurements and PLIF measurements in the y-direction. The resulting interfacial perturbation will take the form of a sum of two Fourier series. The velocity perturbation in the xz-plane will be obtained from w' at the centerline of the mixing layer at a distance $x = 0.75$ cm from the splitter plate. A velocity potential field will be constructed from the spectrum of vertical velocity fluctuations (Drazin & Reid 2004). The two-dimensional velocity field will be extended along the y-axis to form a three-dimensional velocity field. Statistical quantities extracted from both the experiment and simulations will be compared to validate the method of initialization. This numerical investigation is the first use of DNS to model the water channel experiment. These simulations are also the first to use experimentally-measured interfacial and velocity perturbations in all directions.

Another theme present in the numerical simulations is the determination of the quantitative differences between two- and three-dimensional simulations. This work is motivated by the desire to provide more predictive models of experimental flows without the need for computationally expensive three-dimensional calculations. Results will be shown comparing two- and three-dimensional simulations initialized with analogous, experimentally-measured initial conditions. Differences between the results of the simulations will be highlighted and the underlying physical mechanisms that are responsible for these differences will be discussed.

6. Summary

Experiments will be performed to measure the fluctuating density and velocity during the onset of the Rayleigh-Taylor instability in a water channel. Spectra from density, velocity and interfacial fluctuations will be parameterized so that numerical simulations of the experiment may be performed. Both DNS and experimental results will be used to examine the effect of initial conditions on the dynamics of a Rayleigh-

Taylor mixing layer. Of particular interest is the early-time transition of the mixing layer from a weakly-nonlinear to a strongly-nonlinear flow. This work is largely motivated by the desire to develop and evaluate predictive turbulent transport models of buoyancy-driven turbulent flows with an emphasis on the flows that occur in astrophysical and ICF applications.

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References

Adrian, R. J. 1991 Particle-imaging techniques for experimental fluid mechanics. Ann. Rev. Fluid Mech. 23, 261-304.

Andrews, M. J. 1986 Turbulent mixing by Rayleigh-Taylor instability. Ph.D. thesis. Imperial College, London.

Anuchina, N. N., Kucherenko, Y. A., Neuvazhaev, V. E., et al. 1978 Turbulent mixing at an accelerating interface between liquids of different densities. Izv. Akad Nauk. SSSR, Mekh. Zhidk. Gaza 6, 157-160.

Boris, J. P., Grinstein, F. F., Oran, E. S. & Kolbe, R. L. 1992 New insights into large eddy simulation. Fluid Dyn. Res. 10, 199-228.

Cabot, W. H., Schilling, O. & Zhou, Y. 2004 Influence of subgrid scales on resolvable turbulence and mixing in Rayleigh–Taylor flow. Phys. Fluids 16, 495-508.

Chandrasekhar, S. 1961 Hydrodynamic and Hydromagnetic Stability. Dover.

Cook, A. W. & Dimotakis, P. E. 2001 Transition stages of Rayleigh-Taylor instability between miscible fluids. J. Fluid Mech. 443, 69-99.

Cook, A. W., Cabot, W. & Miller, P. L. 2004 The mixing transition in Rayleigh-Taylor instability. J. Fluid Mech. 511, 333-362.

Dalziel, S. B., Linden, P. F. & Youngs, D. L. 1999 Self-similarity and internal structure of turbulence induced by Rayleigh-Taylor instability. J. Fluid Mech. 399, 1-48.

Dimonte, G., Youngs, D. L., Dimits, A. et al. 2004 A comparative study of the turbulent Rayleigh-Taylor (RT) instability using high-resolution 3D numerical simulations: The Alpha-Group collaboration. Phys. Fluids 16, 1668-1693.

Dimotakis, P. E. 2000 The mixing transition in turbulent flows. J. Fluid Mech. 409, 69-98.

Drazin, P. G. & Reid W. H. 2004 Hydrodynamic Stability. 2nd Ed. Cambridge University Press.

Emmons, H. W., Chang, C. T., & Watson, B. C. 1960 Taylor instability of finite surface waves. J. Fluid Mech. 7, 177-193.

Kukulka, D. J. 1981 Thermodynamic and transport properties of pure and saline water. M.S. dissertation, State University of New York at Buffalo.

Lindl, J. D. 1998 Inertial Confinement Fusion: The Quest for Ignition and Energy Gain Using Indirect Drive. AIP Press.

Pope, S. B. 2000 Turbulent Flows. Cambridge University Press.

Pratt W. K. 1991 Digital Image Processing 2nd Ed. Wiley-Interscience.

Ramaprabhu, P. & Andrews, M. J. 2004a Experimental investigation of Rayleigh-Taylor mixing at small Atwood numbers. J. Fluid Mech 502, 233-271.

Ramaprabhu, P. & Andrews, M. J. 2004b On the initialization of Rayleigh-Taylor simulations. Phys. Fluids 16, L59-L62.

Rayleigh, L. 1883 Investigation of the equilibrium of a incompressible heavy fluid of variable density. Proc. London Math Soc. 14, 170.

Read, K. I. 1984 Experimental investigation of turbulent mixing by Rayleigh-Taylor instability. Physica D 12, 45-58.

Smarr, L., Wilson, J. R., Barton, R. T. & Bowers, R. L. 1981 Rayleigh-Taylor overturn in super-nova core collapse. Astrophys. J. 246, 515-525.

Taylor, G. I. 1950 The instability of liquid surfaces when accelerated in a direction perpendicular to their planes. Proc. Royal Soc. London 201, 192.

van Oord, J. 1997 The design of a stereoscopic DPIV-system. Delft University of Technology Report MEAH-161.

Wilson, P. N. & Andrews, M. J. 2002 Spectral measurements of Rayleigh-Taylor mixing at low-Atwood number. Phys. Fluids A 14, 938-945.

Youngs, D. L. 1984 Numerical simulations of turbulent mixing by Rayleigh-Taylor instability. Physica D 12, 32-44.

Youngs, D. L. 1991 Three-dimensional numerical simulations of turbulent mixing by Rayleigh-Taylor instability. Phys. Fluids A 3, 1312-1320.